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14. ABSTRACT

A tandem mass spectrometer incorporating radio-frequency octopole ion guides has been designed, constructed, and tested. This instrument is capable of measuring absolute integral cross sections for gas-phase ion molecule reactions as functions of the reactant's relative translation energy from thermal to hyperthermal energy (0.03 - 20 eV c.m.), and of the neutral reactant's temperature from 298 – 1000 K. A series of calibration studies have been carried out to verify the operating characteristics of this new instrument.

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Final Report

AFOSR DEPSCoR Grant

#F49620-96-1-0409

PI: Peter M. Hierl

1. Objectives

The objectives of this project were (1) to design, build, and test a new instrument for the measurement of absolute integral cross sections of ion-molecule reactions as functions of reactant translational energy and of neutral reactant temperature; and (2) to perform such measurements on several electron-transfer and proton-transfer reactions relevant to the high-temperature plasma surrounding vehicles re-entering the earth's atmosphere.

2. Status of Efforts

A tandem mass spectrometer for the measurement of absolute integral cross sections of ion-molecule reactions at high temperatures has been designed, built, and successfully tested in a series of calibration experiments. Work has begun (and is still in progress) on using this instrument to study selected ion-molecule reactions relevant to the high-temperature plasma surrounding vehicles re-entering the earth's atmosphere.

3. Accomplishments

The major accomplishment has been the design and construction of a tandem mass spectrometer which incorporates octopole ion guides to transmit the reactant ion beam through a high-temperature collision cell containing the neutral reactant, and to transmit reactant and product ions to the detector. The details of this device are given below:

The instrument consists of three differentially-pumped vacuum chambers: an ion source, a reaction region, and an analyzer region. These chambers are pumped by an 1800 L/s diffusion pump, a 5000 L/s diffusion pump, and a 550 L/s turbomolecular pump, respectively. Background pressures in these three regions are ~5×10^{-8} torr, and operating pressures are less than 2×10^{-7} torr.

The reactant ions are generated by electron impact on a precursor gas in a low-pressure source, extracted and focused into a beam which passes at moderate energy (20-100 eV) through a small magnetic sector mass spectrometer. The emerging mass-selected beam is focused by a second

electrostatic lens system into a nearly monoenergetic beam whose energy can be varied from ~0.1-100 eV.

This beam is then injected into the first of two coupled octopole ion guides (i.e., eight parallel rods in a circular array on which opposite phases of a radiofrequency (rf) voltage are applied, thereby creating a confining electric field which guides the ions along the axis of the rods). While traversing the first ion guide (30 cm long), the ions pass through a variable-temperature (298-1000 K) collision cell containing the neutral reactant gas, the pressure of which (typically, ~0.2 mtorr) is measured with a capacitance manometer.

Upon exiting the first octopole ion guide, product ions and transmitted primary ions immediately enter a second octopole ion guide (60 cm long) which is used to measure the translational energy of the ions. To date, we have used a continuous ion beam and performed the energy analysis by using the second octopole as a retarding potential analyzer. It is also possible, however, to pulse the ion beam and use the second octopole as a time-of-flight energy analyzer.

Ions exiting the second ion guide are focused onto the entrance of a quadrupole mass spectrometer for identification. Detection utilizes an electron multiplier and standard pulse counting techniques. The instrument is interfaced with a desktop computer for control of the experimental parameters and for data acquisition.

The operating characteristics of the instrument have been determined in a series of calibration experiments. The instrument was found capable of producing intense (0.5-2 x 10^6 cps), nearly monoenergetic (FWHM = 0.15-0.20 eV) mass selected ion beams over the range of laboratory energies 0.1-100 eV. Integral cross sections were measured at room temperature for a number of well-known ion-molecule reactions; our results were found to be in excellent agreement with data previously published by other authors. For the reaction $Ar^+ + D_2 \rightarrow ArD^+ + D$, measurements were also made at temperatures up to 900 K; the results, corrected for the effects of thermal transpiration, confirmed the proper operation of the instrument at elevated temperatures. In another set of experiments, cross sections were measured for several endoergic ion-molecule reactions (e.g., $Ne^+ + CO \rightarrow Ne + C^+ + O$). The translational energy thesholds observed were in excellent agreement with the known thermodynamic thresholds, indicating both the accuracy of our energy measurements and the utility of this technique for determining such values.

4. Personnel Supported:

Yousef Basir (postdoctoral student, 18 months)
Nadya Galeva (postdoctoral student, 6 months)

5. Publications: none at this time

6. Interactions

a. Participation:

During the period covered in this report, I have been a regular participant at the Molecular Dynamics Contractor's Reviews sponsored by AFOSR, and at Gordon Research Conferences on gas-phase ion chemistry.

b. Consultative/advisory functions

During this project I have visited and consulted with several colleagues (Rainer Dressler, Robert Morris, Albert Viggiano, Skip Williams, and others) at the Air Force Research Laboratory, Hanscom AFB, MA. The subjects discussed included design features of the guided ion beam tandem mass spectrometer, specific ion chemistry relating to the current project, and the possibility of continued collaboration in the future (e.g., ion-enhanced combustion of hydrocarbon fuels).

I have also visted Professors Scott Anderson and Peter Armentrout (University of Utah), and Professor Richard Zare (Stanford University) to discuss the design of this instrument, and have received visits from Rainer Dressler (AFRL) and Professors Kent Erwin (University of Nevada at Reno) and Dieter Gerlich (Technical University of Chemnitz, Germany) for similar discussions.

7. New discoeries: none at this point

8. Honors/Awards: none at this point